

# Semiclassical Approximation for Periodic Potentials

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## Abstract

We derive the semiclassical WKB quantization condition for obtaining the energy band edges of periodic potentials. The derivation is based on an approach which is much simpler than the usual method of interpolating with linear potentials in the regions of the classical turning points. The band structure of several periodic potentials is computed using our semiclassical quantization condition.

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## 1. Introduction

The study of periodic potentials is of both physical and mathematical interest. For instance, in condensed matter physics, knowledge of the existence and locations of band edges and band gaps of periodic potentials is very important for determining many physical properties. Although many general mathematical properties of the eigenstates are known [1], unfortunately, even in one dimension, there are very few analytically solvable periodic potential problems.

One of very successful methods in numerous applications in physics and mathematics is the semiclassical approach. The semiclassical WKB approximation for one dimensional potentials with two classical turning points is discussed in most quantum mechanics textbooks [2]. It was originally proposed for obtaining approximate eigenvalues in the limiting case of large quantum numbers. It has been successfully used for many years to determine eigenvalues and to compute barrier tunneling probabilities. The analytic properties of the WKB approximation have been studied in detail from a purely mathematical point of view, and the accuracy of the method has been tested by comparison between analytic and numerical results [3, 4, 5]. There has been a special surge of interest in recent years due to the development of the supersymmetric WKB method [6, 7, 8].

In this paper, we generalize the standard WKB approach to treat periodic potentials. We derive a new semiclassical quantization condition whose solutions give the energy band edges of periodic potentials. Our derivation is considerably simpler than the standard approach which makes use of connection formulas [9] to match the WKB solutions in classically allowed regions with the solutions in classically forbidden regions. In the usual approach, one makes a linear approximation to the potential in the regions around the

classical turning points where the semiclassical first order WKB wave function diverges. Although the connection formulas resulting from the usual approach turn out to be simple enough, the derivation is quite tedious. Our simpler approach effectively amounts to matching the values and derivatives of the zeroth order WKB wave function which is non-divergent at the classical turning points [10, 11].

In Sec. 2, we describe and justify our simpler approach by first re-deriving the standard WKB quantization condition for potentials on the infinite real line with two classical turning points. The extension to periodic potentials of period  $L$  is given in Sec. 3, the main result being the quantization condition Eq. (16). To the best of our knowledge, this result and our method of derivation have not been previously discussed, even though the semiclassical approximation and periodic potentials have both been studied for many years. In order to check the accuracy of the semiclassical approach, we consider applications to the well-studied class of Lamé potentials  $V(x) = ma(a+1)\text{sn}^2(x, m)$ , where  $\text{sn}(x, m)$  is a Jacobi elliptic function [12]. This is a good choice, since it is one of the very few potentials for which the band edges are analytically known for integer values of  $a$  [13, 14, 15]. A comparison of band edge energies obtained from our WKB quantization condition with exact results is given in Sec. 4. The limitations and successes of the WKB approach for periodic potentials are discussed.

## 2 Simpler Derivation of the Usual WKB Condition

In this section, we look at the standard situation of a potential on the entire real line, which has two classical turning points  $x_L$  and  $x_R$  given by  $V(x) = E$  for any choice of energy  $E$ . From now on, for simplicity, we restrict our attention to symmetric potentials  $V(x) = V(-x)$ . For this case,  $x_L = -x_R$ , and it is sufficient to just look at the half line  $x > 0$ , since the eigenfunctions will be necessarily symmetric or antisymmetric. To derive the WKB quantization condition we have to connect the solution in the classically allowed region with the solution in the classically forbidden region. For the symmetric case, the zeroth order WKB approximation to the wave function for  $x > 0$  is

$$\psi_I^{(0)}(x) = A \cos[\chi(x) - \chi(0)] \quad (1)$$

in the classically allowed region  $x_L \leq x \leq x_R$  and

$$\psi_{II}^{(0)}(x) = B e^{-\chi(x) + \chi(x_R)} \quad (2)$$

in the classically forbidden region  $x > x_R$ . We are using the notation

$$\chi(x) \equiv \frac{1}{\hbar} \int^x p(x, E) dx, \quad (3)$$

where  $p(x, E) = \sqrt{2m|E - V(x)|}$  is the generalized momentum. Matching the wave functions  $\psi_I^{(0)}(x)$  and  $\psi_{II}^{(0)}(x)$  and their first derivatives at  $x_R$  gives two equations

$$A \cos[\chi(x_R) - \chi(0)] = B, \quad (4)$$

$$A \sin[\chi(x_R) - \chi(0)] = B, \quad (5)$$

which yield  $\tan[\chi(x_R) - \chi(0)] = 1$ , or

$$\frac{1}{\hbar} \int_0^{x_R} p(x, E) dx = \frac{1}{4}\pi, \frac{5}{4}\pi, \frac{9}{4}\pi, \dots \quad (6)$$

Similarly for the antisymmetric case, the zeroth order WKB approximation to the wave function for  $x > 0$  is  $\psi_I^{(0)}(x) = A \sin[\chi(x) - \chi(0)]$  in the classically allowed region  $x_L \leq x \leq x_R$  and  $\psi_{II}^{(0)}(x) = B e^{-\chi(x) + \chi(x_R)}$  in the classically forbidden region  $x > x_R$ . Matching these wave functions and their first derivatives at  $x_R$  now gives  $\tan[\chi(x_R) - \chi(0)] = -1$ , or

$$\frac{1}{\hbar} \int_0^{x_R} p(x, E) dx = \frac{3}{4}\pi, \frac{7}{4}\pi, \frac{11}{4}\pi, \dots \quad (7)$$

Combining Eqs. (6) and (7), the quantization condition is

$$\frac{1}{\hbar} \int_0^{x_R} p(x, E) dx = \frac{\pi}{2} \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots \quad (8)$$

which is the usual WKB result for a symmetric potential [2]. The derivation given above is evidently much simpler than the usual textbook approach for deriving connection formulas. However, some comments, explanation and justification of the method used is needed for several points. The usual approach makes use of first order WKB wave functions  $\psi^{(1)}(x) = \psi^{(0)}(x)/\sqrt{p(x)}$ , which diverge at the classical turning points. Although this divergence is understandable in the classical limit, since a classical particle has zero speed at the turning points, it is certainly not present in a full quantum mechanical treatment. Since  $\psi^{(1)}(x)$  is singular, it is necessary to resort to connection formulas and somewhat tricky matching of the wave function  $\psi^{(1)}(x)$  and its first derivative [9], that eventually yields the well known WKB quantization condition Eq. (8).

Why our simple procedure for matching  $\psi^{(0)}(x)$  is justified? Clearly, the correct approach is neither to match  $\psi^{(0)}(x)$  nor  $\psi^{(1)}(x)$ , but to keep a sufficient number of higher order contributions in  $\hbar$ , so that the resulting wave function is non-divergent [11]. This has to be the case, since there is no divergence in the full wave function. A simple way in which the divergence gets tamed is for the WKB wave function to have the form  $\psi^{WKB}(x) = \psi^{(0)}(x)/[\sqrt{p(x)} + \hbar f(x, \hbar)]$ , where  $f(x, \hbar)$  is an analytic function of  $x$  and  $\hbar$ . It is easy to check that requiring  $\psi^{WKB}(x)$  and its derivatives to be continuous amounts to our procedure of matching the value and slope of  $\psi^{(0)}(x)$  at the classical turning point  $x_R$ , which justifies our simple approach.

### 3 Generalization to Periodic Potentials

For a potential with period  $L$ , one is seeking solutions of the Schrödinger's equation subject to the Bloch condition

$$\psi(x) = e^{ikL} \psi(x + L), \quad (9)$$

where  $k$  denotes the crystal momentum. The spectrum shows energy bands whose edges correspond to  $kL = 0, \pi$ , that is the wave functions at the band edges satisfy  $\psi(x) = \pm\psi(x + L)$ . For periodic potentials, the band edge energies and wave functions are often called eigenvalues and eigenfunctions, and we will also use this terminology. A general property of the eigenfunctions for a potential with period  $L$  is the oscillation theorem [1] which states that the band edge wave functions arranged in order of increasing energy have periods  $L, 2L, 2L, L, L, 2L, 2L, \dots$

For any periodic potential, it is sufficient to consider just one period of width  $L$ , say the interval  $[-\frac{L}{2}, \frac{L}{2}]$ . In this paper, we are discussing analytic potentials with  $V_{min}$  and  $V_{max}$  as the minimum and maximum values. Further, we are only looking at symmetric potentials  $V(x) = V(-x)$ , which necessarily makes  $x = 0$  a maximum or minimum. Let us take the origin  $x = 0$  to be at  $V_{min}$ . The eigenfunctions will either be symmetric (S) or antisymmetric (A) about  $x = 0$ . Furthermore, it is easy to see that the potential is also symmetric about  $x = \frac{L}{2}$ , since periodicity and symmetry about  $x = 0$  imply that  $V(x + \frac{L}{2}) = V(-x + \frac{L}{2})$ . Consequently,  $x = \frac{L}{2}$  is an extremum, and the eigenfunctions are necessarily symmetric or antisymmetric about  $x = \frac{L}{2}$ . Clearly, there are four types of eigenfunctions (S,S), (A,S), (S,A), (A,A), where the first letter denotes symmetry or antisymmetry about the origin, and the second letter denotes symmetry or antisymmetry about the point  $x = \frac{L}{2}$ . Note that (S,S) and (A,A) wave functions have period  $L$ , whereas (A,S) and (S,A) wave functions have period  $2L$ . The ground state, being nodeless, is of type (S,S).

To obtain the WKB quantization condition for a periodic potential, consider any energy  $E$  which gives two classical turning points  $x_L$  and  $x_R$  in the interval  $[-\frac{L}{2}, \frac{L}{2}]$ . Since we are looking at symmetric potentials, clearly  $x_L = -x_R$ , and one only needs to look at the half-interval  $[0, \frac{L}{2}]$ . Note that the region  $|x| \leq x_R$  is classically allowed (region I) whereas the region  $x_R < |x| \leq \frac{L}{2}$  is classically forbidden (region II). Let us now derive the WKB quantization condition corresponding to the four eigenfunction types.

For the (S,S) case, the zeroth order WKB approximation to the wave function is given by Eq. (1) in region I and

$$\psi_{II}^{(0)}(x) = B \cosh[-\chi(x) + \chi(L/2)] \quad (10)$$

in region II, where  $\chi(x)$  is defined by Eq. (3). Matching the wave functions  $\psi_I^{(0)}(x)$  and  $\psi_{II}^{(0)}(x)$  and their first derivatives at  $x_R$  gives

$$A \cos[\chi(x_R) - \chi(0)] = B \cosh[-\chi(x_R) + \chi(L/2)], \quad (11)$$

$$A \sin[\chi(x_R) - \chi(0)] = B \sinh[-\chi(x_R) + \chi(L/2)], \quad (12)$$

which, on division, give the equation

$$\tan \left[ \frac{1}{\hbar} \int_0^{x_R} p(x, E) dx \right] = \tanh \left[ \frac{1}{\hbar} \int_{x_R}^{\frac{L}{2}} p(x, E) dx \right]. \quad (13)$$

Similarly, for the (A,S), (S,A) and (A,A) cases, we take zeroth order WKB wave functions with appropriate symmetry

$$(A, S) : \quad \begin{aligned} \psi_I^{(0)}(x) &= A \sin[\chi(x) - \chi(0)], \\ \psi_{II}^{(0)}(x) &= B \cosh[-\chi(x) + \chi(L/2)], \end{aligned}$$

$$(S, A) : \quad \begin{aligned} \psi_I^{(0)}(x) &= A \cos[\chi(x) - \chi(0)], \\ \psi_{II}^{(0)}(x) &= B \sinh[-\chi(x) + \chi(L/2)], \end{aligned}$$

$$(A, A) : \quad \begin{aligned} \psi_I^{(0)}(x) &= A \sin[\chi(x) - \chi(0)], \\ \psi_{II}^{(0)}(x) &= B \sinh[-\chi(x) + \chi(L/2)], \end{aligned}$$

and match wave functions and their first derivatives at  $x_R$ . Combining all results gives

$$\tan \left[ \frac{1}{\hbar} \int_0^{x_R} p(x, E) dx \right] = \pm \tanh \left[ \frac{1}{\hbar} \int_{x_R}^{\frac{L}{2}} p(x, E) dx \right], \quad (14)$$

$$\tan \left[ \frac{1}{\hbar} \int_0^{x_R} p(x, E) dx \right] = \pm \coth \left[ \frac{1}{\hbar} \int_{x_R}^{\frac{L}{2}} p(x, E) dx \right]. \quad (15)$$

Taking into account the periodicity of  $\tan \chi(x)$ , we can write a single combined equation

$$\frac{1}{\hbar} \int_0^{x_R} p(x, E) dx = \frac{\pi}{2} n \pm \arctan \left[ \tanh \left( \frac{1}{\hbar} \int_{x_R}^{\frac{L}{2}} p(x, E) dx \right) \right]. \quad (16)$$

This is our final semiclassical WKB quantization condition for symmetric periodic potentials of period  $L$ , the solutions to which are the WKB band edge energies  $E_n^{WKB}$ . The quantum number  $n$  takes on non-negative integer values which keep the right hand side of Eq. (16) positive. Eq. (16) is a generalization of the usual two classical turning points quantization condition of Eq. (8), which is found in quantum mechanics textbooks. This can be readily established, since when  $L \rightarrow \infty$ ,  $\tanh \left[ \frac{1}{\hbar} \int_{x_R}^{\frac{L}{2}} p(x, E) dx \right]$  tends to unity, and one gets Eq. (8).

## 4 Applications and Discussion

In order to study the accuracy of band edges resulting from the WKB quantization condition derived in the previous section, we consider several examples. These are selected from the class of Lamé potentials

$$V(x) = ma(a+1) \operatorname{sn}^2(x, m), \quad (17)$$

where the Jacobi elliptic function  $\text{sn}(x, m)$  has period  $4K(m)$ . The potentials have a period  $L = 2K(m)$ . It is well known that for any integer value  $a = 1, 2, 3, \dots$ , the corresponding Lamé potential has  $2a + 1$  band edges corresponding to  $a$  bound bands followed by a continuum. All band edge eigenfunctions are analytically known [13, 14, 15].

The Lamé potential given in Eq. (17) has  $V_{min} = 0$  and  $V_{max} = ma(a + 1)$ . A comparison of exact, analytically available band edge energies with results obtained from the WKB quantization condition applied to a variety of Lamé potentials is shown in Table 1.

The quantum number  $n$  and the symmetry of the wave functions about the points  $x = 0$  and  $x = \frac{L}{2}$  are also tabulated. The results are consistent with the pattern required by the oscillation theorem for periodic potentials [1]. Note that for  $m = 1$ , the period of the Lamé potentials becomes infinite and all finite bands reduce to zero width. This feature, which is evident for the exact energies of the potential  $V = 12 \text{sn}^2(x, 1)$  considered in Table 1, is also reproduced in the WKB approach. Also, in Table 1, it should be noted that some exactly known band edges occur above  $V_{max}$ . For example, choosing  $a = 2, m = 0.5$ , one has the potential  $V(x) = 3 \text{sn}^2(x, 0.5)$ . It has two energy bands ranging from 1.27 to 1.50 and from 3.0 to 4.5, with a continuum above 4.73. Clearly, the band edges above  $V_{max} = 3$  cannot be obtained by the semiclassical WKB method, since there are no classical turning points for  $E > V_{max}$ . This is a limitation of the semiclassical approach. However, for  $V_{min} \leq E \leq V_{max}$ , it is apparent from Table 1 that results obtained from our WKB quantization condition are in modest agreement with exact band edge eigenenergies.

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Table 1: Exact and WKB band edge energies.

Potential	$E_n^{\text{exact}}$	$E_n^{\text{WKB}}$	$n$	Symmetry
$3 \text{ sn}^2(x, 0.5)$	1.27	1.34	0	S,S
	1.50	1.96	1	A,S
	3.00	2.81	1	S,A
	4.50	-	-	-
	4.73	-	-	-
$6 \text{ sn}^2(x, 0.5)$	2.05	2.19	0	S,S
	2.13	2.35	1	A,S
	5.05	4.95	1	S,A
	6.00	-	-	-
	6.95	-	-	-
	9.87	-	-	-
	9.95	-	-	-
$9.6 \text{ sn}^2(x, 0.8)$	2.68	2.87	0	S,S
	2.68	2.87	1	A,S
	7.04	7.10	1	S,A
	7.20	7.49	2	A,A
	9.32	9.12	2	S,S
	10.52	-	-	-
	10.96	-	-	-
$12 \text{ sn}^2(x, 1)$	3.00	3.21	0	S,S
	3.00	3.21	1	A,S
	8.00	8.14	1	S,A
	8.00	8.14	2	A,A
	11.00	11.07	2	S,S
	11.00	11.07	3	A,S
	12.00	12.07	3	S,A

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